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A mathematical model of carbon dioxide transport in concrete carbonation process

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1 Introduction

Concrete carbonation is known as one of a phenomenon which is a big serious damage to concrete buildings. From the civil engineering point of view, its analysis of the dynamics is very important problem. In the paper, we report some mathematical results for a model of carbon dioxide transport in this phenomenon without the precise proof.

First, we explain the concrete carbonation phenomenon. Concrete is harding of sand, gravel with cement, and the main ingredient of cement is calcium hydroxide $Ca(OH)_2$ which shows alkalinity. The exposure concrete always touchs air, and carbon dioxide CO_2 enters the porous structure of concrete-based materials, and CO_2 dissolves in the pore water by Henry's law. Since $Ca(OH)_2$ also dissolves in this pore water, CO_2 reacts with available alkaline species $Ca(OH)_2$, i.e.

$$Ca(OH)_2 + CO_2 \to CaCO_3 + H_2O \quad \text{in pore water.}$$

In this reaction, by OH^- is comsumed, alkalinity changes into acidly. In the case of the reinforced concrete, by this phenomenon, there is rust forming on the surface of the iron bar in the concrete, and by the volume expanding of the iron bar, the crack is formed. Therefore, the concrete carbonation gives a big effect to the durability and the persistence of the concrete buildings.

On a mathematical result of concrete carbonation, Muntean-Böhm [14] considered a mathematical model of concrete carbonation process as a free boundary problem of the carbonated front in one dimensional case, and proved the existence and uniqueness of a solution of this problem. Also, Aiki-Muntean [5, 6] considered a reduction model of Muntean-Böhm, and proved the large time behavior of the free boundary. Our aim of this study is to construct a mathematical model of this process in three dimensional

case and to analyze the dynamics of concrete carbonation process. As the first step of this study, Aiki-Kumazaki [1, 3] proposed a mathematical model of moisture transport which contains the hysteresis operator due to Maekawa-Ishida-Kishi[13] and Maekawa-Chaube-Kishi [12], and proved the existence and uniqueness of a solution of this model. For the uniqueness of a solution of this model, Aiki-Krejči-Kumazaki [4] proved in three dimensional case by using various techniques of [11].

In the paper, we focus on the carbon dioxide in this process. In [2, 8], we proposed the following balanced law of carbon dioxide transport due to Maekawa-Chaube-Kishi [12] and Maekawa-Ishida-Kishi [13]:

$$\frac{\partial}{\partial t}\{\phi(z)[(1-\mathcal{S})v+\mathcal{S}u]\}-\mathrm{div}(\phi(z)[\mathcal{H}_1(1-\mathcal{S})\nabla v+\mathcal{H}_2\mathcal{S}\nabla u]) = -\kappa uw \text{ in } Q(T) := (0,T)\times\Omega, \tag{1.1}$$

and

$$w(t) = w(0)e^{-\tilde{\kappa}\int_0^t u(\tau)d\tau}u(t),\ z(t) = 1 - e^{-\tilde{\kappa}\int_0^t u(\tau)d\tau} \text{ for } t > 0. \tag{1.2}$$

From the physical point of view, Ω is a domain occupied by concrete, and the unknown functions $v = v(t,x)$ and $u = u(t,x)$ represent the concentration of carbon dioxide in air and the concentration of carbon dioxide in water at a time t and a position $x \in \Omega$, respectively. In the equilibrium state, it is known that the relation $v = \rho_0 u$ holds for a positive constant ρ_0 by Henry's law. Also, $\phi = \phi(z)$ represents the porosity, which is the ratio of the volume of the total pore spaces inside of concrete to the volume of the whole concrete, and z is the ratio of the volume of consumed calcium hydroxide to the volume of the total calcium hydroxide. Moreover, $\mathcal{S}$ represents the degree of saturation corresponding to the relative humidity, and the relationship between the relative humidity and the degree of saturation is given as a hysteresis operator in [12, 13]. In the flux term, $\mathcal{H}_1$ and $\mathcal{H}_2$ are positive constants. In the forcing term, κ is a reaction rate and w represents the concentration of calcium ion and this forcing term represents the consumed carbon dioxide in the concrete carbonation process, and is given by the reaction rate theory.

Here, we show that w and z has the form of (1.2) briefly. From the reaction rate theory we have

$$\frac{d}{dt}[\mathrm{CaCO_3}] = \kappa[\mathrm{Ca^{2+}}][\mathrm{CO_3^{2-}}], \tag{1.3}$$

where $\mathrm{Ca^{2+}}$ and $\mathrm{CO_3^{2-}}$ are calcium ion and carbonate ion, respectively. Next, we assume that

$$\rho_1[\mathrm{Ca(OH)_2}] + \rho_2[\mathrm{CaCO_3}] = \text{constant}. \tag{1.4}$$

Here, ρ_1 and ρ_2 are molecule weight of calcium hydroxide and molecule weight of calcium carbonate, respectively. The relation (1.4) is based on the mentioned above chemical reaction in concrete carbonation process. Now, we consider $[\mathrm{Ca(OH)_2}]$ and u as $[\mathrm{Ca^{2+}}](=w)$ and $[\mathrm{CO_3^{2-}}]$ in water, respectively. Then, by the time-derivative of (1.4) and (1.3) we have the following ordinary differential equation:

$$\frac{d}{dt}[\mathrm{Ca^{2+}}] = -\kappa\frac{\rho_2}{\rho_1}[\mathrm{Ca^{2+}}][\mathrm{CO_3^{2-}}].$$

By solving this equation and using the relation $[CO_3^{2-}] = u$ we have the form of w in (1.2). Therefore, by z is the ratio of the volume of consumed calcium hydroxide to the volume of the total calcium hydroxide, namely, $([Ca^{2+}](0) - [Ca^{2+}])/[Ca^{2+}](0)$, we have the form of z in (1.2). Since it is difficult to deal with the equation (1.1) directly, as the first step of this research, we studied the following simplified equation with the boundary and initial condition:

$$\frac{\partial}{\partial t}[\phi(1 - e^{-\int_0^t u(\tau)d\tau}) \cdot u] - \Delta u = -w_0 u e^{-\int_0^t u(\tau)d\tau} \quad \text{in } Q(T) := (0,T) \times \Omega, \tag{1.5}$$

$$u = u_b \quad \text{on } S(T) := (0,T) \times \partial\Omega, \tag{1.6}$$

$$u(0) = u_0 \quad \text{in } \Omega, \tag{1.7}$$

where u_b is a given function on $Q(T)$, and w_0 and u_0 are given functions on Ω. In this paper, we show the existence and uniqueness of a time global solution of the problem (P)=$\{(1.5), (1.6), (1,7)\}$ and the large time behavior of that solution.

2 Mathematical results

2.1 Existence and uniqueness of a solution

In this section, we show the existence and uniqueness of a solution of (P). First, we assume the following items:

(A1) $\Omega \subset \mathrm{R}^3$ is a bounded domain with a smooth boundary $\Gamma = \partial\Omega$.

(A2) ϕ is a non-decreasing function in $\mathrm{C}^1(\mathrm{R})$ such that $c_0 = \sup_{r\in\mathrm{R}} \phi'(r) < \infty$ and $\phi_0 \le \phi(r) \le 1$ for $r \in \mathrm{R}$ and a positive number ϕ_0.

(A3) $u_b \in W^{1,2}(0,T; H^1(\Omega)) \cap L^\infty(0,T; H^2(\Omega))$ and $0 \le u_b \le \kappa_0$ in $Q(T)$ for a positive number κ_0.

(A4) $u_0 \in H^1(\Omega) \cap L^\infty(\Omega)$, $u_0 \ge 0$ in Ω and $u_0 = u_b(0)$ on $\partial\Omega$.

(A5) $w_0 \in L^\infty(\Omega)$ and $w_0 \ge 0$ in Ω.

Next, we define a solution of (P) on $[0,T]$ in the following way:

Definition Let u be a function on $Q(T)$ for $0 < T < \infty$. We call that the function u is a solution of (P) on $[0,T]$ if the following conditions (S1) $\sim$ (S4) hold:

(S1) $u \in W^{1,2}(0,T; H) \cap L^\infty(0,T; H^1(\Omega)) \cap L^2(0,T; H^2(\Omega))$, and $u \ge 0$ a.e. on $Q(T)$.

(S2) $[\phi(1 - e^{-\int_0^t u(\tau)d\tau}) \cdot u]_t - \Delta u = -w_0 u e^{-\int_0^t u(\tau)d\tau}$ a.e. in $Q(T)$.

(S3) $u = u_b$ a.e. on $S(T)$.

(S4) $u(0) = u_0$ in Ω.

Then, the following existence and uniqueness of (P) holds.

Theorem 1. (Kumazaki [8]) *Under the assumptions (A1) $\sim$ (A5), for any $T > 0$, (P) has one and only one solution u on $[0,T]$ such that*

$$0 \le u \le u^* \text{ a.e. on } Q(T),$$

where u^* is a positive constant depending on the boundary and initial data.

2.2 Large time behavior of a solution

Large time behavior of a solution, in particular the convergences of a solution of (P) to a solution of the steady state problem of (P) is important to see that how much the concrete is carbonated finally. In fact, by $0 \leq u$ a.e. on $Q(T)$ in Theorem 1 $v(t) = e^{-\int_0^t u(\tau)d\tau}$ is decreasing with respect to t so that we see that there exists a limit of $v(t)$ as $t \to \infty$. If we can show that $v(t) \to 0$ a.e. on Ω as $t \to \infty$, then $1 - v(t) = 1 - e^{-\int_0^t u(\tau)d\tau} \to 1$ as $t \to \infty$ for a.e. $x \in \Omega$. Since z is the ratio of the volume of consumed calcium hydroxide to the volume of the total calcium hydroxide, $z = 1$ a.e. on Ω implies that calcium hydroxide is fully consumed at almost everywhere in the concrete. Accordingly, finally, we see that the concrete is carbonated at almost everywhere.

On this subject, we assume the same condition in Theorem 1 except the condition (A3), and impose the following condition (A3)' instead of (A3):

(A3)' $u_b \in L^\infty(0,\infty;H^2(\Omega))$ with $0 \leq u_b \leq \kappa_0$ in Ω for a positive number κ_0 and $(u_b)_t \in L^2(0,\infty;H^1(\Omega)) \cap L^1(0,\infty;H^2(\Omega))$. Also, there exists $u_{b\infty} \in H^2(\Omega)$ such that $u_b - u_{b\infty} \in L^2(0,\infty;H^1(\Omega))$.

Next, we note that the steady state problem $(\mathrm{P})_\infty$ of (P) is as follows:

$$-\Delta u_\infty + \phi'(1-w_\infty)w_\infty u_\infty^2 = -w_0 u_\infty w_\infty \text{ in } \Omega,$$

$$u_\infty = u_{b\infty} \text{ on } \Gamma,$$

where $u_{b\infty}$ is a given function in Ω which is a limit of u_b as $t \to \infty$ and $w_\infty = w_\infty(x)$ is a limit of $w(x,t) = \exp\left(-\int_0^t u(x,\tau)d\tau\right)$ as $t \to \infty$, namely, $w(x,t) \to w_\infty(x)$ as $t \to \infty$ for each $x \in \Omega$. The existence of a solution of $(\mathrm{P})_\infty$ can be obtained by using the maximal monotone theory by Barbu [7]. Also, it is easy to see that $0 \leq u_\infty \leq u_\infty^*$ a.e. on Ω where u_∞^* is a positive constant depending on the initial data. Our result concerning about the convergences to a solution of $(\mathrm{P})_\infty$ is as follows:

Theorem 2. (Kumazaki [9]) *Assume (A1) (A2) (A3)' (A4) and (A5) hold, and let u and u_∞ be a solution of (P) and $(P)_\infty$, respectively. Then,*

$$u(t) \to u_\infty \textit{ strongly in } L^2(\Omega) \textit{ and weakly in } H^1(\Omega) \textit{ as } t \to \infty.$$

Moreover, we can obtain the following results for two cases of $u_{b\infty}$.

Corollary 1. (Kumazaki [9]) *Assume (A1), (A2), (A3)' (A4) and (A5) hold, and let u and u_∞ be a solution of (P) and $(P)_\infty$, respectively. Then,*

(i) if $u_{b\infty}$ does not vanish identically on Γ, then u_∞ is a solution of the following steady state problem

$$-\Delta u_\infty = 0 \textit{ a.e. in } \Omega, \quad u_\infty = u_{b\infty} \textit{ a.e. on } \Gamma.$$

Also, $w_\infty = 0$ a.e. on Ω.

(ii) if $u_{b\infty} = 0$ *a.e. on* Γ, *then* $u_\infty = 0$ *a.e. on* Ω. *Moreover, if* $u_b = u_{b\infty} = 0$ *a.e. on* Ω, *then, there exists a positive constant* α *such that*

$$|u(t)|_H^2 \leq |u_0|_H^2 e^{-\alpha t} \quad \text{for } t \geq 0.$$

The first result of Corollary 1 implies that the concrete is carbonated at almost everywhere, finally. In the second result of Corollary 2, although it is not usual situation, we show the convergence rate to a solution of $(\mathrm{P})_\infty$. In the case of (i) of Corollary 1, the following decay rate hold by restricting the boundary data:

Theorem 3. (Kumazaki [10]) *Assume the same condition (A1), (A2), (A3)', (A4) and (A5) in Theorem 2 hold, and let* u *and* u_∞ *be a solution of (P) and* $(P)_\infty$, *respectively. In addition, we assume that* $u_b \geq \kappa$ *in* Ω *for a positive constant* κ *satisfying* $(\phi_0 C_P^2)^{-1} > \kappa$ *where* C_P *is a positive constant by Poincaré's inequality. Then, there exists* $t^* > 0$ *such that*

$$|u(t) - u_\infty|_H^2 \leq Ce^{-\kappa t} \quad \text{for } t > t^*,$$

where C *is a positive constant.*

In Theorem 3, the condition $u_b \geq \kappa$ in Ω is very important to derive the above decay rate, and in (i) of Cororally 1, the above decay rate could not be obtained by the lack of this condition. Also, we can see that the decay rate depends on the size of the domain, namely, the size of the concrete.

However, the above results is one of the simplified version of the original problem so that a lot of open problem still remain on this problem. In particular, we try to consider the original model of carbon dioxide transport with the following more realistic boundary condition:

$$\frac{\partial u}{\partial n} = C(u - u_b) \text{ on } S(T),$$

where n is the outer unit normal vector on the boundary and C is a positive constant. If C is sufficiently large, then we can consider this condition as the same imhomogenious Dirichlet boundary condition (1.4).

In future, we try to consider the system consisting of (1.1) and a parabolic equation which represents a mathematical model of moisture transport handled in [1, 3] as a mathematical model of concrete carbonation phenomenon.

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